Focus Report

New Chemicals Program

Case Number: P-13-0248

Focus Date: 02/21/2013

Report Status: Complete

Focus Chair: Darlene Jones

Contractor: Legacy Placeholder

Consolidated Set:

I. Notice Information

Submitter: [redacted]

CAS Number: 171611-11-3

Chemical Name: Imidodisulfuryl fluoride, lithium salt (1:1)

Use: [redacted]

Other Uses: [redacted]

Bind: ☐ **imports:** ☑

Manufacture: ☐ **PV-max(kg/yr):** [redacted]

II. SAT Results

Health Rating 1: 2 **Health Rating 2:**

Occupational Rating: 2-3B **Non Occupational Rating:** 3

Ecotox Rating 2: **Environmental Rating:** 2

Health Rating Comment 1:

Health Rating Comment 2:

Persistence 1: 3 **Bioaccumulation 1:** 1 **Toxicity 1:** 2

PBT Comments 1:

III. OTHER FACTORS

Categories

Health Chemical Category:

Ecotox SARs: lithium salts

Ecotox SAR Class: [redacted]

Ecotox TSCA New Chemical Category: None

Related Cases / Regulatory History

Health Related Cases:

Ecotox Related Cases: [redacted]

Regulatory History: [redacted]

MSDS/Label Information

MSDS: Y **Label:** N

General Equipment: rubber or polyethylene gloves/ protective glasses, goggles, protective face shield / use closed equipment/machinery or use local ventilation equipment.

Respirator: Dust mask, NIOSH certified particulate respirator.

Health Effects: Toxic if swallowed. Causes severe skin burns. Causes serious eye damage. The dust can form an explosive mixture.

TLV/PEL(PMN or raw material): - Lithium Salt - 99 % - as particulate not otherwised regulated. OSHA PEL-TWA (2009) - Lithium Salt - 99 % - as particulate not otherwised regulated. ACGIH TLV-TWA (2009)

LVE PPE:

Exposure Based Information

Exposure Based Review (Chemistry): Y

Exposure Based Review (Health): N

Exposure Based Review (Ecotox): Y

Exposure Based Review (Occupational): Y

Exposure Based Review (Non-Occupational): N

Exposure Based Review (Environmental):

IV. Summary of SAT Assessment

Fate

Fate Summary: P-13-0248
FATE:
[redacted] with MP = [redacted] (M)
S = [redacted] (M)
[redacted]
POTW removal (%) = 0; OECD 301C (MITI): 2% (BOD)/28d NRB; OECD 305 (Biocon): under detectable limit: <11-fold(low), <1-fold(high)/28d.
Time for complete ultimate aerobic biodeg > mo
Sorption to soils/sediments = low
PBT Potential: P3B1
*CEB FATE: Migration to ground water = rapid

Ecotox

Ecotox Values

Fish 96-h LC50: 540(P) >100(M)

Daphnid 48-h LC50: 120(P) 71(M)

Green Algae 96-h EC50: 780(P) >100(M)

Fish Chronic Value: 6.7(P) >10(M)

Daphnid Chronic Value: 1.6(P) 7.1(M)

Green Algae Chronic Value: 190(P) 70.7(M)

Ecotox Value Comments: Predictions are based on SARs for lithium salts; SAR chemical class = lithium salt with [redacted] Li; [redacted]); pH7; effective concentrations based on 100% active ingredients and mean measured concentrations; hardness <150.0 mg/L as CaCO3; and TOC <2.0 mg/L;

Ecotoxicity Test Data Results for P-13-0248: Imidodisulfuryl fluoride, lithium salt (1:1)
(CASRN: 171611-11-3; [redacted].

Acute ecotoxicity tests were conducted with fish, daphnia, and algae in 2010 on P-13-0248 by Nisso Chemical Analysis Service Co., Ltd (Japan) for [redacted]. The PMN material was a colorless and transparent liquid with an estimated vapor pressure of <1 x 10-6 mm Hg at 25 °C. The measured water solubility of the PMN material is 500 g/L at 25 °C. The sorption to soils and sediments is low and the time to complete ultimate aerobic biodegradation is estimated to be greater than months. These studies complied with OECD guidelines for: 1) O2, pH, temperature, water hardness values and other water quality parameters; 2) species, age, number of organisms per replicate, and biomass loading rates; and, 3) replicate and overall variability. The tests were performed in a GLP laboratory and a quality assurance statement provided for each test.

Fish Ecotoxicity Test:
Nisso Chemical Analysis Service Co., Ltd conducted a 96-hour acute toxicity study in Medaka (Oryzias latipes) with P-13-0248 (solid content: 24.0% aqueous solution) under semi-static conditions (48-hour renewal cycle). The study was reported to follow the "Testing Methods for New Chemical Substances" (November 21, 2003; No. 1121002, Pharmaceutical and Food Safety Bureau, Ministry of Health, Labour and Welfare). Following the results of a range-finding study, a single replicate of seven O. latipes was exposed to a dilution water control (dechlorinated tap water) or the PMN substance at a nominal concentration of 100 mg/L (initial measured concentration of 103 mg/L). To prepare the 100 mg/L test solution, 300 mg of the test substance (1249.8 mg as aqueous solution) was weighed and transferred to a 1000-mL volumetric flask and dissolved in dechlorinated tap water. This solution was transferred into the test chamber and then added 2 L dechlorinated water to prepare the exposure solution. The test substance concentrations in the test solutions ranged from 99.0 to 103% of the nominal concentration during the exposure period, according to LC/MS/MS analysis. Throughout the exposure period, no turbidity or precipitate was observed and the test solutions were clear and transparent. Over the course of testing, temperature was maintained at 22.8 – 22.9 ˚C, pH ranged from 7.4-8.0, and dissolved oxygen ranged from 6.5-8.0 mg/L. Dilution water hardness was 60 mg CaCO3/L. A loading rate of 0.23 g fish/L was calculated. No mortality or abnormal responses were observed during the exposure; therefore, the 96-hour LC50 is greater than 100 mg/L (nominal concentration).
96-hour LC50 > 100 mg/L

Daphnid Ecotoxicity Test:
Nisso Chemical Analysis Service Co., Ltd conducted a 48-hour test in water fleas (Daphnia magna) with P-13-0248 (solid content: 24.0% aqueous solution) under static conditions. The study was reported to follow the "Testing Methods for New Chemical Substances" (November 21, 2003; No. 1121002, Pharmaceutical and Food Safety Bureau, Ministry of Health, Labour and Welfare). Following the results of a range-finding study, four replicates of five daphnids were exposed to a dilution water control (dechlorinated tap water) or the PMN test substance at nominal concentrations of 6.26, 12.5, 25.0, 50.0, and 100 mg/L. Corresponding initial measured concentrations of 6.48, 12.7, 25.5, 53.0, and 105 mg/L (102 – 106% of nominal) were determined by LC/MS/MS analysis. To prepare the test solutions, an amount of test substance (417 mg as aqueous solution; 100 mg as LiFSI) was weighed and transferred at a 1000-mL volumetric flask and dissolved in dechlorinated tap water (two solutions were prepared, one was for stock solution and another was for the test solutions). The stock solutions (31.3, 62.5, 125 and 250 mL) were separately transferred to 500-mL flasks and brought to volume with dechlorinated tap water to prepare the test solutions of 6.26, 12.5, 25.0, and 50.0 mg/L, respectively. All test solutions in the exposure and control groups were colorless and transparent during the exposure period. At the end of the exposure period, measured concentrations were determined to be 6.12, 12.3, 25.3, 49.3, and 98.0 mg/L (97.8 – 101% of nominal). Over the course of testing, temperature was maintained at 19.6-19.7 ˚C, pH ranged from 7.8-7.9, and dissolved oxygen ranged from 7.3-9.1 mg/L. Dilution water hardness was 55 mg CaCO3/L. A loading rate of 50 daphnids /L was calculated. Abnormal behavior was observed during the exposure duration in the nominal concentrations of 25, 50, and 100 mg/L. One hundred percent immobilization was observed in the highest nominal test concentration resulting in a 48-hour EC50 of 71 mg/L (nominal concentration).
48-hour EC50 = 71 mg/L

Algal Ecotoxicity Test:
Nisso Chemical Analysis Service Co., Ltd conducted a 72-hour growth inhibition study in green algae (Pseudokirchneriella subcapitata) with P-13-0248 (solid content: 24.0% aqueous solution) under static conditions. The study was reported to follow the "Testing Methods for New Chemical Substances" (November 21, 2003; No. 1121002, Pharmaceutical and Food Safety Bureau, Ministry of Health, Labour and Welfare). Following the results of a range-finding study, six replicates of P. subcapitata (5000 cells/mL) were exposed to a dilution water (OECD medium) control and three replicates were exposed to the PMN substance at nominal concentrations of 6.25, 12.5, 25.0, 50.0, and 100 mg/L. Algae were illuminated at a light intensity ranging from 69 – 86 µE/m2/s with constant shaking. The test solutions were prepared by adding the test substance (624.9 mg; 150 mg as LiFSI) to a 300-mL volumetric flask and dissolved in the OECD medium and the volume was adjusted to prepare a 500 mg/L stock solution. The stock solutions (6.25, 12.5, 25.0, 50.0 and 100 mL) were separately transferred to 500-mL flasks and filled to volume with OECD medium to prepare the test solutions. The concentrations of the test substance in the test solutions were 104-106% of the nominal at the exposure initiation and 99.6-103% of the nominal at the exposure termination, according to LC/MS/MS analysis. Due to problems with the control growth rate in the definitive test, a second definitive test was conducted. The first definitive test was not used by the testing laboratory. The results of the first definitive test were not included in the algal submission. The information provided in this 72-hr algal toxicity test review only reflects results from definitive test number two. The concentrations were stable during the exposure period. Over the course of testing, temperature was maintained at 22.9-23.0 °C, and the pH ranged from 7.9-8.1. The cell density in the control increased by a factor of 172 after 72 hours. The 72-hour EC50 for growth rate is > 100 mg/L. Abnormal algal shapes were observed in the highest test concentration (nominal 100 mg/L). The NOEC and LOEC for growth rate are 50 and 100 mg/L, respectively, and the ChV (geometric mean of the NOEC and LOEC) is 70.7 mg/L.
72-hour EC50 (growth rate) > 100 mg/L
72-hour NOEC = 50 mg/L
72-hour LOEC = 100 mg/L
72-hour ChV = 70.7 mg/L

Conclusions:
The fish (96-hour LC50 > 100 mg/L), daphnia (48-hour EC50 = 71 mg/L), and algal (72-hour EC50 (growth rate) > 100 mg/L and 72-hour ChV = 70.7 mg/L) toxicity studies are acceptable for P-13-0248. For comparative purposes, the fish (96-hr LC50), acute daphnia (48-hr EC50), and algal (96-hr EC50) toxicity values, based on SARs for P-13-0248, are 540 mg/L, 120 mg/L, and 780 mg/L, respectively. In addition, based on the same SAR equations, the fish, daphnia, and algal chronic values for P-13-0248 are 6.7 mg/L, 1.6 mg/L, and 190 mg/L, respectively.
The acute concentration of concern (CoC) is calculated by dividing the 48-hr acute toxicity value for D. magna by an uncertainty factor of 5 yielding 14,200 ppb (71,000 µg/L / 5). The fish and daphnia chronic values for P-13-0248 are calculated dividing their experimental acute toxicity values by an acute to chronic ratio (ACR) of 10. The fish and aquatic invertebrate chronic values for P-13-0248 are > 10 mg/L and 7.1 mg/L, respectively. The chronic concentration of concern for P-13-0248 is calculated by dividing the lowest aquatic chronic value (D. magna-7.1 mg/L) by an uncertainty factor of 10 yielding 710 µg/L or 710 ppb.

The acute CoC = 14,200 ppb
The chronic CoC = 710 ppb

Ecotox Study Reviewer: J. Gallagher
February 13, 2013

Ecotox Factors

Acute Aquatic Factors:	**Most Sensitive Endpoint:**	**Assessment Factor:** 10	**CoC:**
Chronic Aquatic Factors:	**Most Sensitive Endpoint:**	**Assessment Factor:**	**CoC:** 710

Comments:

V. Summary of Exposure/Releases

Engineering Summary Release

Exposures/Releases	**Release**	**Release**
Scenario	[redacted]	[redacted]
Site	[redacted]	[redacted]
Media	[redacted]	[redacted]

Exposures/Releases	Release	Release	
Descriptor A	Output 2	Output 2	Conservative
Quantity A (Release=kg/site/day; Exposure=mg/day)	[redacted]	[redacted]	[redacted]
Frequency A (day/year)	[redacted]	[redacted]	[redacted]
Descriptor B			
Quantity B (Release=kg/site/day; Exposure=mg/day)			
Frequency B (day/year)			
From	[redacted]	[redacted]	[redacted]
Workers			
ExposureType			

Exposures/Releases	Exposure	Exposure	
Scenario	[redacted]	[redacted]	[redacted]
Site	[redacted]	[redacted]	[redacted]
Media	Dermal	Dermal	Inhalation
Descriptor A	High End	High End	Upper Bound
Quantity A (Release=kg/site/day; Exposure=mg/day)	[redacted]	[redacted]	[redacted]
Frequency A (day/year)	[redacted]	[redacted]	[redacted]
Descriptor B			
Quantity B (Release=kg/site/day; Exposure=mg/day)			
Frequency B (day/year)			
From	[redacted]	[redacted]	[redacted]
Workers	30	30	30
ExposureType	[redacted]	[redacted]	[redacted]

Exposures/Releases	Release	Release	
Scenario	[redacted]	[redacted]	U M
Site	3	3	3
Media	[redacted]	[redacted]	D
	High End	Conservative	

Exposures/Releases	Release	Release	
Descriptor A			H E
Quantity A (Release=kg/site/day; Exposure=mg/day)	[redacted]	[redacted]	5
Frequency A (day/year)	[redacted]	[redacted]	2
Descriptor B			
Quantity B (Release=kg/site/day; Exposure=mg/day)			
Frequency B (day/year)			
From	[redacted]	[redacted]	U fr D
Workers			9
ExposureType			L

Exposure Summary Release

Chemical ID: P-13-0248

Reviewer: YX-Exposure-Based 5(e)

Exposure Scenario	Water						Land fill (non-sludge)	Stack	
Release Activity(ies) exposure Calculations	Drinking Water		Fish Ingestion						
	ADR mg/kg/day	LADD mg/kg/day	ADR mg/kg/day	LADD mg/kg/day	7Q10cc ug/l	PDM Exceeded # Days	LADD mg/kg/day	ADR mg/kg/day	LAD mg/kg/
PROC: Max LADD	0.00e+0	0.00e+0	0.00e+0	0.00e+0	0.00e+0	0.00e+0	0.00e+0	0.00e+0	3.16E-0
USE: Max LADD	0.00e+0	0.00e+0	0.00e+0	0.00e+0	0.00e+0	0.00e+0	0.00e+0	0.00e+0	3.59E-0

[redacted]

Result Table : Exposure Based(XB)/Persistent (P2B2) Criteria

Parameter	Exp Based	Persistent	
Drinking(Surface) Water Dose (mg/kg/day)	No	NA	
Fish Ingestion Dose (mg/kg/day)	No	NA	
Inhalation Dose (mg/kg/day)	No	NA	
Groundwater Dose (mg/kg/day)	No	NA	
Surface Water Release After Treatment (kg/yr)	No	NA	

Parameter	Exp Based	Persistent
Total Release After Treatment (kg/yr)	No	NA
Consumer Use?	No	

VI. Focus Decision and Rationale

Regulatory Actions

Regulatory Decision: PMN Standard Review **Decision Date:** 02/25/2013

Decision Type:

Rationale: P-13-0248 was placed into standard review to review all human health test data and for exposure-based ecotoxicity concerns. A T.I., full team, and schedule will be needed for the review process. Human health hazard concerns were moderate for inhalation and dermal exposures. The submitter must remove the use of a dust-mask from the MSDS. Appropriate respiratory protection equipment will be determined during the review process. Ecotoxicity hazard concerns were moderate based on submitted test data for lithium salts. Potential risks to the environment were low due to less than 20 days of exceedences of the COC during the release period, however due to exposure-based ecotoxicity concerns the required ecotoxicity testing will be the daphnid chronic toxicity test (OPPTS Test Guidelines 850.1300). The following CEB exposure-based criteria were met: # of workers exposed: 1,345 >1000 and Routine Dermal Cont: >250 workers & >100 days/yr. The following EAB exposure-based criteria were met: [redacted]

COC: Chronic – 710 ppb, Acute – 14,200 ppb

Summary of Exposures and Releases

Proc
[redacted]
Inhalation (Particulate): [redacted]
Dermal: [redacted]
Dermal: [redacted])

Releases to Water: [redacted]
Or Air or Incineration or Landfill
Releases via Incineration: [redacted]
Releases via Incineration: [redacted]

Fate Releases to Air:
Stack Air: LADD: [redacted]
Fugitive Air: LADD: [redacted]

Fate Releases to Water (Removal Rate 0%):
SWC: [redacted]
DW: LADD: [redacted]
>COC (710 ppb) [redacted]

Use
[redacted]
Inhalation: negligible (VP < 0.001 torr)
Dermal: [redacted]

Releases to Water: [redacted]
Or Incineration or Landfill
Releases to Water: [redacted]
Or Incineration or Landfill

Fate Releases to Water (Removal Rate 0%):
SWC: [redacted]
DW: LADD: [redacted]
>COC (1 ppb) [redacted]

Use
Fate Releases to Water (Removal Rate 0%):
SWC: [redacted]
DW: LADD: [redacted]

P2 Rec Comments:

Testing

Health:

Ecotox:

Fate:

Final Recommendations